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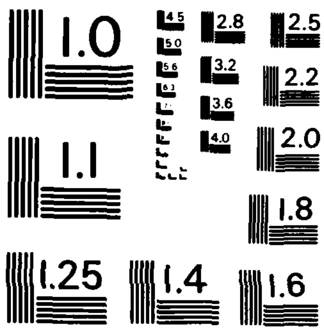
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

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20. ABSTRACT CONTINUED

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THE STRUCTURE OF DEFECTS IN GaAs AND RELATED MATERIALS

FINAL REPORT

C.B. CARTER

AUGUST 24, 1985

U.S. ARMY RESEARCH OFFICE

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ABSTRACT

The principal reasons which necessitate an extensive study of dislocations and grain boundaries in GaAs and related compound semiconductors are briefly reviewed. Dislocations may be present in the substrate material which is used in the growth of epi-layer structures, or may be introduced during growth as occurs in strained-layer systems, or they may be generated during operation of the device. In this program a new approach for characterizing super-lattice stuctures has been developed which uses REM to examine the layer quality rather than conventional TEM. The technique developed by Alexander to deform Si at low temperatures has been applied for the first time to GaAs. The resulting dislocation structure consists of a high density of very straight screw dislocations lying accurately along their Peierls valleys. The dislocation are immobile until irradiated in the electron beam, whereupon the alpha-dislocations glide away at very high speeds. This glide is therefore a recombination-enhanced process. The rate of motion depends strongly on the character (screw, 60°, or edge) and nature (alpha- or beta-) of the dislocation. It has also been shown that it depends on the order of the partial dislocations and on their character. The results are complimentary to those of Maeda and Takeuchi, but are at much higher spatial resolution. This technique has been extended to the technologically important case of the superlattice by actually deforming a series of superlattice structures at these same low (150°C) temperatures. Finally a new approach has been developed for growing bicrystals of GaAs using a Ge bicrystal as a substrate.

Background

The purpose of this report is to summarise the progress which has been made as a result of the present program. The report will detail the initial aims of the program as defined in the original proposal and will indicate to what extent these specific tasks have been completed. As the program has progressed, some side issues of direct relevance to the overall aim of the research have also been investigated in a preliminary way. Much of this research has developed from a strong collaboration with Prof.L.F. Eastman's research group at Cornell.

The principal defects studied have been dislocations and grain boundaries, since each is highly suitable for detailed analysis by transmission electron microscopy (TEM). The necessity for detailed analysis of these defects in III-V compound semiconductors has grown significantly during the four years since the program was initially proposed. Amongst the principal reasons for this study are the following:

a) Large numbers of dislocations are, at present, unavoidable and possibly advantageous in the bulk GaAs used for substrate material.

b) Devices degrade during operation due to the formation of dislocation tangles which can act either as electrical short circuits or, in the case of LEDs, as centers for non-radiative recombination.

c) Dislocations are often present at the heterojunctions between different compound semiconductors. Although these dislocations are present in order to accommodate lattice misfit, it does appear that they can propogate into individual layers. This effect may be due, in part, to a change in lattice parameters as the layers cool from the growth temperature.

d) There is considerable interest in strained-layer superlattices. The principle involved in the growth of such materials is that misfit dislocations will not form providing the layers are sufficiently thin. Observations suggest that this ideal situation is not usually achieved and may, for large numbers of layers, be intrinsically impossible. The misfit strain energy is lowered by generation of such defects.

e) Metallization contacts to GaAs may also induce local stresses which may then punch out dislocations.

f) Grain boundaries may appear to have very little direct relevance to dislocations. However, the work on grain boundaries in Si and Ge has produced a revolution in our understanding of dislocations in these materials; it is believed to be equally likely that new information will be produced on dislocations in GaAs since, for example, the dislocations can belong to the α- or β-set, in addition to being on either the glide or shuffle planes.

Methods of Approach

The approach followed in this program has been twofold. Firstly, interactions have been developed with Profs Lester Eastman and Joseph Ballantyne in the School of Electrical Engineering at Cornell, which have led to extensive studies of superlattices, quantum-well structures, doping effects, grain boundary structures and metallization effects. In the study of metal contacts to GaAs an extensive collaboration with Prof. Jim Mayer in our own department has begun.

Secondly, deformation experiments have been carried out not only at higher temperatures (~400°C) but also at temperatures as low as 150°C. The initial worry was that deformation experiments would be difficult because GaAs decomposes incongruently at temperatures above 550°C. This decomposition has proved not to be a problem at 400°C and is certainly negligible at 150°C.

As detailed in the original proposal all aspects of TEM have been used to characterize the dislocations. The electrical properties of the dislocations have, to date, only been studied indirectly as relates to the α- or β-character. However, model systems have now been developed and we have been approached by several groups, who specialise in the determination of electrical properties, with a view to providing such model samples for in depth characterization. Of the several possible future interactions those with Prof. J.W. Steeds at Bristol University, England, who has developed a new high-resolution, CL (cathodo-luminescence) technique, and Dr. D.B. Holt, at Imperial College in London, who has a system for both CL and EBIC (electron-beam induced current), are particularly exciting.

Results

A) *Development of New Techniques*

i) We have developed a new technique for the study of superlattices and quantum-wells in compound semiconductors. The technique uses reflection electron microscopy (REM) in the TEM in a manner similar to that used for studying surfaces. The new advance is both in the specimen preparation method and the ability to differentiate between areas which differ chemically (eg. GaAs and $Al_xGa_{1-x}As$). The principle of the technique is that a superlattice structure is cleaved normal to the [001] growth direction and examined by "reflecting" electrons from the surface, thus avoiding the time-consuming process of preparing a TEM sample. The chemical information is obtained because dark-field images in REM are structure-factor sensitive just as they are in conventional TEM.

ii) We have developed a new technique for deforming GaAs in a controlled manner at low temperatures under high-stress following the approach used by Alexander for Si.

iii) We have developed a new technique for growing bicrystals of GaAs by using a Ge bicrystal as the substrate.

B) ***New Results***

i) Controlled deformation of GaAs has led to several very important new results and the promise of new advances in the future. Samples deformed at low temperatures (150°C) contain dislocations which lie predominantly along their <110> Peierls valleys. However, during observation in the TEM, these dislocations can move rapidly. In fact, the α-dislcoations move so quickly that it has not been possible to record images of most of those observed. In future, it is hoped that low-dose TEM techniques will be successful using a video camera, image intensifier and image processing system for image enhancement. At both the low (150°C) and higher (400°C) temperatures we have produced strings of dislocation loops. This observation is intriguing since it suggests that pipe diffusion may be important at very low temperatures in GaAs. At the higher temperatures we have formed large numbers of faulted dipoles even under deformation by single slip. This result is again interesting and important for several reasons. Faulted dipoles are model defects for the study of stacking-faults and dislocation cores, as has been shown by analogous studies in Ge and Si. Furthermore, such devices as LEDs are thought to degrade by the formation of dislocation dipoles and yet very little information is available on dislocation dipoles in GaAs.

ii) The deformation of GaAs at 150°C has led to new information on the mechanism and rate of dislocation glide in GaAs. For the first time it has been shown directly for GaAs that electron-hole recombination can influence the mobility of individual partial dislocations and dislocation kinks in GaAs. These direct observations compliment and extend the observations by Maeda and Takeuchi of dislocation movement in the SEM.

iii) The interaction of dislocations with heterojunctions is important for many reasons. It has, for example, been proposed that superlattices should be included in epilayer structures as a barrier to dislocations present in the substrate. Dislocations are also often present within superlattice structures, particularly in strained-layer superlattices. Models for the formation of misfit dislocations are simply inadequate. For example, none of the available models gives a satisfactory, consistent explanation of the density of misfit dislocations. A new approach which has produced intriguing results has been developed in this program. The idea is to deform a superlattice or quantum-well structure in single slip at a low temperature (150°C) and then cut the sample parallel to one of the primary glide planes. The result is that the dislocations can be very thoroughly characterized since they are several microns long and their interaction with the heterojunctions can be studied by rotating the specimen to view the interface edge-on. One surprising result of this study is that dislocation dipoles are often produced by dislocations gliding through superlattice structures. This observation is clearly important in relation to the degradation of GaAs-based devices.

iii) A closely-related study has been begun as part of this program in a collaboration with Lester Eastman's group. Its aim is to understand the origin of ion-damage in superlattices. It has been shown by this preliminary study that when the ion-implanted superlattice is annealed, dislocation loops form. In GaAs/$Al_xGa_{1-x}As$ superlattices these loops form primarily in the GaAs layers! We have proposed a model wherein the dislocation loops nucleate at the heterojunction and locally relieve the lattice mismatch since the dislocation loops are primarily interstitial in nature. The similarity to the dislocation/heterojunction is then striking.

iv) Our study of grain boundaries began to bear fruit during the last 6 months of this program and has produced several new insights. It should be remembered that although grain boundaries are important defects in themselves, they also provide a unique approach to the detailed study of dislocations. Although Holt's pioneering theoretical analysis is now 20 years old, there have been few direct observations of grain boundaries in GaAs. The present study has produced new observations on first-, second- and third-order twins and on the $\Sigma=5$ high-angle boundary. Faceting of all of these interfaces is common. We also have obtained preliminary observations on low-angle, tilt boundaries and their interaction with antiphase boundaries. In fact, our observations on antiphase boundaries and their faceting has found immediate application. Understanding antiphase boundaries is not only important in view of the interest in growing polar materials on non-polar substrates or layers (eg. GaAs on Ge) but such defects also provide the first direct method of examining antisite bonding, i.e. As-As or Ga-Ga. In view of the importance of anti-site defects to the EL2 defect, this new advance holds great potential significance.

v) Since the doping of III-V compounds is very important in the actual application of these materials, we have included aspects of this topic in our program through our collaboration with Lester Eastman. The major results obtained in this area have been a) a new insight into the growth of Si doped $Al_xGa_{1-x}As$, b) a new understanding of how Sn "rides the surface" during MBE-growth of Sn-doped GaAs, and c) a new awareness of some of the problems and pitfalls in the growth of $Al_xGa_{1-x}As$ by OMVPE.

Detailed references to related work in the literature are given in the publications listed in the following section.

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J: Journals, C: Conference Proceedings

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C69. De Cooman, B.C. and Carter, C.B., 1985, submitted to MRS, ***"TEM Study of the Core-Structure of Dislocations in GaAs".***

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3. ***"Characterization of Semiconductors by TEM"***
   14 June, 1984.
   Upstate NY Chapter of the American Vacuum Society,
   Rochester, NY.

6. ***"Study of III-V Compound Semiconductor Device Structures"***
   13 Nov., 1984.
   Honeywell Corporate Technology Center, Minnesota.

7. ***"Study of III-V Compound Semiconductor Device Structures"***
   15 Jan., 1985.
   Hewlett Packard, Palo Alto, Ca.

8. Discussion Leader: ***Dislocations and Heterojunctions Session,***
   Gordon Research Conference on Point and line defects and
   Interfaces in Semiconductors, 1985.
   Plymouth, New Hampshire.

Personnel who have been supported wholly or in part by this program:

C.B. Carter is the Principal Investigator.

Mr Bruno C. De Cooman has been primarly supported by this program and is due to complete his Ph. D. in summer 1986.

Dr Karl-Heinz Kuesters worked as a post-doctoral associate.

Dr Steven Chen has been supported, in part, by this program through his work on Sn-Doped GaAs. Dr Chen completed his Ph. D. in July 1985 and now works for Eastman-Kodak in Rochester, NY.

Mr Nam-Hee Cho is directly involved in the program but is supported by a fellowship from the Government of South Korea. Mr Cho joined the program as a Ph. D. student in Jan. 1984.

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